



chain nodes :

13 15 16 17 18 19 20 21 22 23 24 25 26 27 28 34 35 36 37 38 39 40

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 14 29 30 31 32 33

chain bonds :

4-13 8-20 10-21 12-25 13-14 13-15 15-16 15-17 17-18 17-19 19-20 21-22 21-23 21-24
25-26 25-27 25-28 31-34 34-35 34-36 36-37 37-38 38-39 39-40

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 14-29 14-33 29-30 30-31
31-32 32-33

exact/norm bonds :

13-14 14-29 14-33 15-16 15-17 17-18 17-19 29-30 30-31 31-32 31-34 32-33 34-35
34-36 38-39

exact bonds :

4-13 8-20 10-21 12-25 13-15 19-20 21-22 21-23 21-24 25-26 25-27 25-28 36-37 37-38
39-40

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

isolated ring systems :

containing 1 : 7 : 14 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:CLASS 14:Atom 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS
21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:Atom
30:Atom 31:Atom 32:Atom 33:Atom 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS
40:CLASS